Malhotra Day 18. The Schrödinger Equation (Ctd.)

The Hamiltonian Operator:

Classically Hamiltonian is a function of coordinates, momenta and time

$$\mathcal{H} \equiv \mathcal{H}(\{q, p\}, t) \quad -(1)$$

For a N-particle system, in most cases, it is conveniently written as a sum of the total kinetic energy of the system and the total potential energy. The latter can arise from both internal interactions and interactions with external forces/fields

$$\mathcal{H} = T(\{p\}) + V(\{q\}, t) \quad -(2)$$

$$T = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} \quad -(3)$$

$$V = V(\{q\}) + \sum_{i=1}^{N} v_{ext}(q_i, t) \quad -(4)$$

(We will see atleast one noteable exception to this later in the course)

Written as in 2, the Hamiltonian tracks the instantaneous total energy of the system. Note that 'q' represent generalized coordinates that are not necessarily the Cartesian coordinates of the particles. The momenta {p} are correspondingly generalized as well.

To keep matters simple, we will initially only focus on Cartesian coordinates and momenta. Using postulate 2, we can promote 3 to a Q.M. operator as:

$$\hat{H}(t) \equiv \sum_{i=1}^{N} \hat{p}_i^2 / 2m_i + V(\{\vec{r}_i\}, t) \quad -(5)$$

In analogy with its identity in classical mechanics, (4) can be thought of as the total energy operator.

Note that $\hat{H}^{\dagger} = \hat{H}$ — (6) i.e. Hermitian

**Postulate 6:** The time evolution of a state of a (quantum) system is determined by the relation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{\mathcal{H}}(t) |\Psi(t)\rangle \quad \text{(7)}$$

Here $|\Psi(t)\rangle$ is presumed to be normalized at all times.

(7) is called the (Time-dependent) Schrödinger Equation, after its author E. Schrödinger. (TDSE)

Usually, we know the state we have prepared the system in. Let's call this as $|\Psi(t=0)\rangle \equiv |\Psi(0)\rangle$. — (8)

$\because$ (7) is a first-order differential equation in time, this one initial condition is sufficient to solve (9), in principle.

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## An aside on differential equation

An equation of the form

$$\sum_{j=0}^{n} p_j(x)\, y^{(j)}(x) = f(x) \quad - \text{①}$$

where $a < x < b \in \mathbb{R}$

$y^{(j)}(x) = \dfrac{d^j}{dx^j} y(x)$ , where $y \in \mathbb{R}$

$\left(\text{s.t } y^{(0)}(x) = y(x)\right)$

is called a linear differential equation

If $n$ is the highest order derivative for which the corresponding function $p_n(x) \neq 0$, then the equation is said to be of $n^{th}$ order.

All the functions $\{p_j(x)\}$, $f(x)$ are presumed to be defined on the open interval $x \in (a, b)$.

If we define the differential operator

$$\hat{\mathcal{L}} \equiv \sum_{j=0}^{n} p_j(x) \frac{d^j}{dx^j} \quad \text{—} (2)$$

then (1) is also written as

$$\hat{\mathcal{L}}\, y(x) = f(x) \quad \text{—} (3)$$

In such a case, since

$$\hat{\mathcal{L}}\,(y_1 + y_2) = \hat{\mathcal{L}} y_1 + \hat{\mathcal{L}} y_2 \quad \text{—} (4)$$

$\hat{\mathcal{L}} \rightarrow$ linear operator,
Hence the term linear D.E.

We often encounter initial value problems where the value of the function $y(x)$ along with that of its derivatives is known at some point $x_0$. We then desire to determine the fn $y(x)$ which satisfies these initial conditions & eq. (3).

Theorem 1 : (Existence & Uniqueness)

Given an $n^{th}$ order LDE (3), along with the auxilliary conditions:

$$y^{(j)}(x_0) = z_j \ , \ j=0,n \ ,$$ if $\{p_j(x)\}_{j=0,n}$ and $f(x)$ are real, finite, single-valued and continous in some region surrounding the point $(x_0, z_0)$ then there is one and only one solution to the LDE. in an interval $-h \leq x_0 \leq h$ lying within the region.

Thus, the existence & uniqueness of a solution, given a set of initial conditions, can be guaranteed.

Let us specialize to the case of $2^{nd}$ order LDE. That is, with

$$\hat{\mathcal{L}} = p_2(x)\, y''(x) + p_1(x)\, y'(x) + p_0(x)\, y(x) = f(x) \quad \text{— (5)}$$

so that

$$\hat{\mathcal{L}}\, y(x) = f(x) \quad \text{— (6)}$$

**Homogenous L.D.E.**: The equation

$$\hat{\mathcal{L}}\, y(x) = 0 \quad \text{— (5)}$$

is called a homogeneous L.D.E.

**Theorem 2**: If $y_1(x)$ is a solution to (5) then so is $c\, y_1(x)$ where $c \in \mathbb{C}$.

**Theorem 3**: If $y_1(x)$ & $y_2(x)$ are any 2 solution of (5) then so is $c_1 y_1(x) + c_2 y_2(x)$ $c_1, c_2 \in \mathbb{C}$.

This is just the principle of superposition of solutions.

Note that since (5) is not accompanied by auxilliary conditions, it is possible to find multiple solutions.

However, it turns out that it is possible to generate all possible solutions from just a few basic ones. The solutions to (5) all form a linear vector space over complex fields. So it is possible to ask how many linearly independent solutions can we find at most. This number is, of course, the dimension of the solution space.

**Theorem 4:** There are $n$ linearly independent solutions possible for a $n^{th}$ order homogeneous L.D.E.
The general solution to the L.D.E. is then of the form:

$$y(x) = c_1 y_1(x) + c_2 y_2(x) + \dots + c_n y_n(x) \qquad — (6)$$

where $\{y_i(x)\}_{i=1,n}$ are a set of $n$ L.I. solutions.

(ie. $\sum_{i=1}^{n} \alpha_i y_i(x) = 0 \Rightarrow \alpha_i = 0 \ \forall i=1,n$ is the only solution)

Linear independence can be checked by computing the Wronskian:

$$W(x) = \begin{vmatrix} y_1 & y_2 & \cdots & y_n \\ y_1^{(1)} & y_2^{(1)} & \cdots & y_n^{(1)} \\ \vdots & & & \\ y_1^{(n-1)} & y_2^{(n-1)} & \cdots & y_n^{(n-1)} \end{vmatrix} \qquad — (7)$$

The functions are L.I if and only if $W(x) \neq 0$ for some $x \in (a, b)$

domain where solution is sought.

$\therefore$ For a $2^{nd}$ order Homogeneous L.D.E. there are at most two linearly independent solutions.